Dichloroacetylene
7572-29-4 | DTXSID7020429

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -65.0 °C

Global applicability domain: Inside

Local applicability domain index: 6.07e-01

Confidence level: 6.01e-01

Nearest Neighbors from the Training Set

Image not found
Dichloroacetylene
Measured: -66.0
Predicted: -65.0

Image not found
1,3,5-Cycloheptatriene
Measured: -79.5
Predicted: -74.2

Image not found
1,3-Cyclopentadiene
Measured: -85.0
Predicted: -83.9

Image not found
1,3,5,7-Cyclooctatetraene
Measured: -4.70
Predicted: -37.8